# Chapter-19
# Infrared spectroscopy
# (Bond Parameter & Hybridization)

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**IR absorption frequency depends on bond properties or bond parameter. Bond strength, masses of the bonded atoms and hybridization state affect the infrared absorption frequency as follows:**

**1. Bond multiplicity: Bond multiplicity of homonuclei species is directly proportional to IR absorption frequency (higher frequency or higher wave number $cm^{-1}$).**

**i.e. Bond multiplicity of homonuclei species α IR absorption frequency**

Eg. C≡C (2150 $cm^{-1}$) > C=C (1650 $cm^{-1}$) > C-C (1200 $cm^{-1}$). Thus Triple bonds (≡) are stronger than double bonds (=) over single (-) bond.

**2. Masses of the bonded atoms: Masses of the bonded atoms are inversely proportional to the IR absorption Frequency.**

**i.e. Masses of the bonded atoms α 1/ IR absorption frequency**

Eg. The C-H stretch occurs at about 3000$cm^{-1}$. As the atom bonded to carbon increases in mass (i.e.atomic weight) then the frequency of vibration decreases (wave numbers $cm^{-1}$ get smaller).

C-H (3000$cm^{-1}$)→C-C (1200$cm^{-1}$)→C-O (1100$cm^{-1}$)→C-Cl (750$cm^{-1}$)→C-Br (600$cm^{-1}$)→C-I (500 $cm^{-1}$)

(At.wt.H -1.008 C – 12.01 O-15.99 Cl-35.45 Br-79.90 I-126.9)

**3. Hybridization: Hybridization affects the IR absorption frequency. With increasing power of the hybridization state ($P_{Hyb}$), IR absorption frequency decreases.**

**i.e. Power of the hybridization state α 1/ IR absorption Frequency**

Eg. Bonds are stronger is in the order sp ($P_{Hyb}$=1) > $sp^2$ ($P_{Hyb}$= 2) > $sp^3$ ($P_{Hyb}$= 3). Thus IR absorption frequency follows the order

≡C-H ($P_{Hyb}$=1, sp, 3300$cm^{-1}$) > =C-H ($P_{Hyb}$= 2, $sp^2$, 3100$cm^{-1}$) > -C-H ($P_{Hyb}$=3, $sp^3$, 2900$cm^{-1}$)

## Related Questions:

***Q.1. Arrange the following into their decreasing order of infrared absorption frequency ($cm^{-1}$)***

**i) $CH_3$-$CH_3$, $CH_2$=$CH_2$, CH≡CH**

**ii) C-Cl, C-I, C-Br**

**iii) C-H, C-O, C-C**

**iv) =C-H, -C-H, ≡C-H**

***Q.2. Which one of the following will have higher IR absorption frequency ($cm^{-1}$)***

**a. C-O** **b. C-C** **c. C-Cl** **d. C-Br**

## Reference Books:

*1. Fourier Transforms in NMR, Optical and Mass Spectroscopy, Alan G. Marshall, Francis R. Verdun, Elsevier, 1990.*

*2. Practical Fourier Transform Infrared Spectroscopy, John R. Ferraro, K. Krishnan, Academic Press, 1990*

*3. Infrared Spectroscopy: Fundamentals and Applications, Barbara H. Stuart, John Wiley & Sons, Ltd, 2004.*

*4. Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A: Theory and Applications in Inorganic Chemistry, Sixth Edition, Kazuo Nakamoto, John Wiley & Sons, Ltd, 2008.*

*5. Infrared and Raman spectroscopy principles and spectral interpretation, Peter Larkin, Elsevier, 2011.*

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